

# SCALAR FIELD DYNAMICS: CLASSICAL, QUANTUM AND IN BETWEEN\*

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Using a Hartree ensemble approximation, we investigate the dynamics of the  $\varphi^4$  model in 1+1 dimensions. We find that the fields initially thermalize with a Bose-Einstein distribution for the fields. Gradually, however, the distribution changes towards classical equipartition. Using suitable initial conditions quantum thermalization is achieved much faster than the onset of this undesirable equipartition. We also show how the numerical efficiency of our method can be significantly improved.

## 1 Inhomogeneous Hartree Dynamics

In many areas of high-energy physics, e.g. heavy ion collisions and early universe physics, a non-perturbative understanding of quantum field dynamics is required. Computer simulations could fulfill this need, but as is well-known the problem is very difficult. Hence one resorts to approximations, such as classical dynamics<sup>1</sup> (for recent work see<sup>2</sup>), large  $n$  or Hartree (see e.g. <sup>3</sup>). Here we introduce and apply a different type of Hartree or gaussian approximation than used previously, in which we use an ensemble of gaussian wavefunctions to compute Green functions. We can only sketch this method here, a detailed presentation will appear elsewhere.

We use the lattice  $\varphi^4$  model in 1 + 1 dimensions as a test model, which has the following Heisenberg operator equations,

$$\dot{\hat{\varphi}} = \hat{\pi}, \quad \dot{\hat{\pi}} = (\Delta - \mu^2)\hat{\varphi} - \lambda\hat{\varphi}^3, \quad (1)$$

with  $\Delta$  the lattice laplacian,  $\mu$  the bare mass and  $\lambda$  the coupling constant. Rather than solving the operator equation (1) in all detail, one may focus on the Green functions. The Hartree approximation assumes that the density matrix used to compute these Green functions is of gaussian form, such that all information is contained in the one- and two-point functions. The one-point function is the mean field and the connected two-point function is conveniently expanded in terms of mode-functions,

$$\langle \hat{\varphi}_x \rangle = \varphi_x, \quad \langle \hat{\varphi}_x \hat{\varphi}_y \rangle_{\text{conn}} = \sum_{\alpha} f_x^{\alpha} f_y^{\alpha*}. \quad (2)$$

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We have restricted ourselves to *pure state* gaussian density matrices here. The Heisenberg equations now provide self-consistent equations for the mean field  $\varphi$  and the mode functions  $f^\alpha$ ,

$$\begin{aligned}\ddot{\varphi}_x &= \Delta\varphi_x - [\mu^2 + \lambda(\varphi_x^2 + 3 \sum_{\alpha} f_x^\alpha f_x^{\alpha*})]\varphi_x \\ \ddot{f}_x^\alpha &= \Delta f_x^\alpha - [\mu^2 + \lambda(3\varphi_x^2 + 3 \sum_{\alpha} f_x^\alpha f_x^{\alpha*})]f_x^\alpha\end{aligned}\quad (3)$$

In order to simulate a more general density matrix than the gaussian ones required in the Hartree approximation, we average over a suitable ensemble of Hartree realizations, by specifying different initial conditions and/or coarsening in time. In this way we may compute Green functions with a non-gaussian density matrix  $\hat{\rho} = \sum_i p_i \hat{\rho}_i^G$ , as

$$\langle \hat{\varphi}_x \hat{\varphi}_y \rangle_{\text{conn}} = \sum_i p_i [\langle \hat{\varphi}_x \hat{\varphi}_y \rangle_{\text{conn}}^{(i)} + \varphi_x^{(i)} \varphi_y^{(i)}] - (\text{disconn.}) \quad (4)$$

Note that the individual Green functions labeled by  $i$  are still computed with pure gaussian states  $\hat{\rho}_i^G$ , as is appropriate in the Hartree approximation.

The field operator in the Hartree approximation may be written as

$$\hat{\varphi}_x = \varphi_x + \sum_{\alpha} [f_x^\alpha \hat{a}_\alpha + f_x^{*\alpha} \hat{a}_\alpha^\dagger], \quad (5)$$

with  $\hat{a}_\alpha$  and  $\hat{a}_\alpha^\dagger$  time-independent creation and annihilation operators. This suggests that the mode functions represent the (quantum) particles in the model. It should be stressed that in general  $\varphi_x$  is *inhomogeneous* in space. We also note that the equations (3) can in fact be derived from a hamiltonian. Since the equations are also strongly non-linear, this suggests that the system will evolve to an equilibrium distribution with equipartition of energy, as in classical statistical physics.

## 2 Observables

To assess the viability of the Hartree ensemble approximation, we solve the equations (3) starting from a number of initial conditions. With Hartree dynamics we expect to go beyond classical dynamics, because the width of the (gaussian) wavefunction, represented by the mode functions, should capture important quantum effects. Of course we cannot expect to capture everything, e.g. tunneling is beyond the scope of the gaussian approximation.

Similarly to using classical dynamics, we expect that after coarse-graining in space and time and averaging over initial conditions, we may compute the

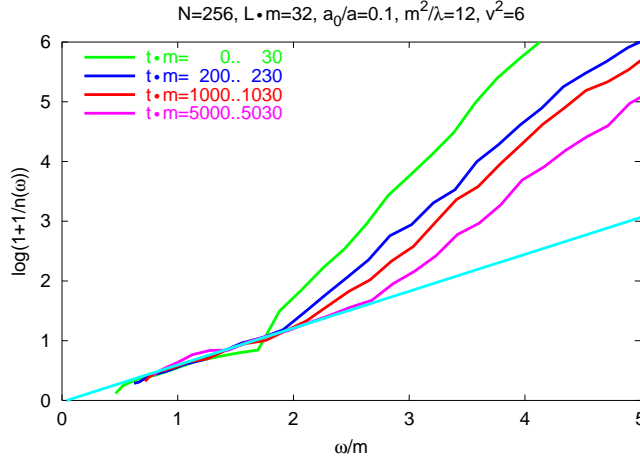


Figure 1. Particle number densities as a function of  $\omega$  at various times. The straight line gives a BE distribution with temperature  $T/m = 1.7$ . (The lattice volume  $Lm = 32$ , coupling  $\lambda/m^2 = 0.083$  and inverse lattice spacing  $1/am = 8$ ;  $m \equiv m(T=0)$ ).

particle number densities and energies from the (Fourier transform of the) connected two-point functions of  $\varphi$  and  $\pi$ ,

$$\frac{1}{N} \sum_{xz} e^{-ikz} \langle \overline{\hat{\varphi}_{x+z} \hat{\varphi}_x} \rangle_{\text{conn}} = \frac{n_k + \frac{1}{2}}{\omega_k}, \quad \frac{1}{N} \sum_{xz} e^{-ikz} \langle \overline{\hat{\pi}_{x+z} \hat{\pi}_x} \rangle_{\text{conn}} = (n_k + \frac{1}{2})\omega_k. \quad (6)$$

The over-bar indicates averaging over some time-interval and initial conditions as in eq. (4),  $\omega_k$  is the energy,  $n_k$  the (number) density of particles with momentum  $k$  and  $N$  the number of lattice sites.

For weak couplings, such as we will use in our numerical work, the particle densities should have a Bose-Einstein (BE) distribution,

$$n_k = 1/(e^{\omega_k/T} - 1), \quad \omega_k = (m^2(T) + k^2)^{\frac{1}{2}}, \quad (7)$$

with  $T$  the temperature and  $m(T)$  an effective finite temperature mass.

### 3 Numerical results

First we use initial conditions which correspond to fields far out of equilibrium: gaussians with mean fields that consist of just a few low momenta modes,

$$\varphi_x = v, \quad \pi_x = A \sum_j^{j_{\max}} \cos(k_j x + \alpha_j). \quad (8)$$

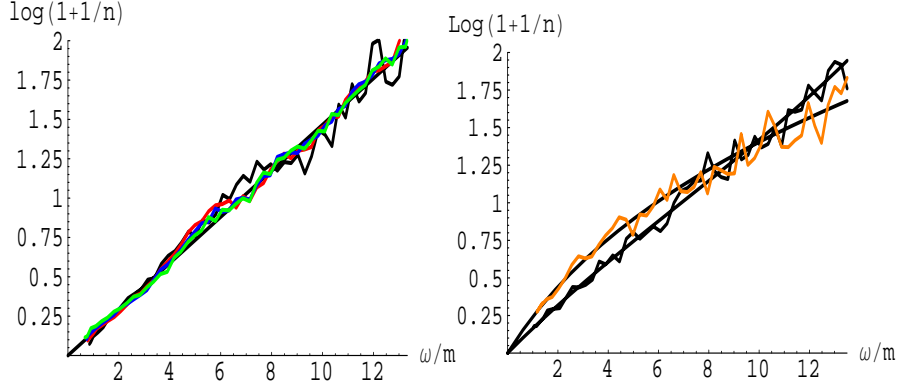


Figure 2. Left: Particle number densities as a function of  $\omega$  at times  $tm = 100, 1400, 2800$  and  $4200$  (bottom up), starting from BE type initial conditions for the mean field. The straight line through the origin is a BE distribution with temperature  $T/m = 6.7$ . The right figure uses classical dynamics and shows data at  $tm = 100$  and  $tm = 4200$ . ( $Lm = 23$ ,  $\lambda/m^2 = 0.083$  and  $1/am = 22$ ).

The  $\alpha_j$  are random phases and  $A$  is a suitable amplitude. Initially the mode functions are plane waves,  $e^{ikx}/\sqrt{2\omega L}$ , i.e. there are no quantum particles and all energy resides in the mean field.

The results in Fig. 1 show that very fast,  $tm \lesssim 200$ , a BE distribution is established for particles with low momenta. Slowly this thermalization progresses to particles with higher momenta, while the temperature  $T \approx 1.7m$  remains roughly constant. Such a thermalization does *not* happen when using *homogeneous* Hartree dynamics ( $\varphi$  constant in space). The difference may be understood, because particles in our method can scatter off the inhomogeneities in the mean field.

Next we want to speed-up the thermalization of the high momentum modes. Therefore we use different initial conditions in which the energy is distributed more realistically over the Fourier modes of the mean field. The modes are the same as before but mean fields are drawn from an ensemble with a BE-like probability distribution,

$$P(\varphi_k, \pi_k) \propto \exp[-(e^{\omega_k/T_0} - 1)(\pi_k^2 + \omega_k^2 \varphi_k^2)/2\omega_k] \quad (9)$$

Now we find density distributions as shown in Fig. 2 (left). Already after a short time,  $tm \approx 100$  the particles have acquired a BE distribution up to large momenta  $\omega/m \approx 12$ . Note that even with these BE-type initial conditions, the fields initially are still out of equilibrium: energy is initially carried by the mean field only but is quickly, within a time span of  $tm \approx 200$ , redistributed

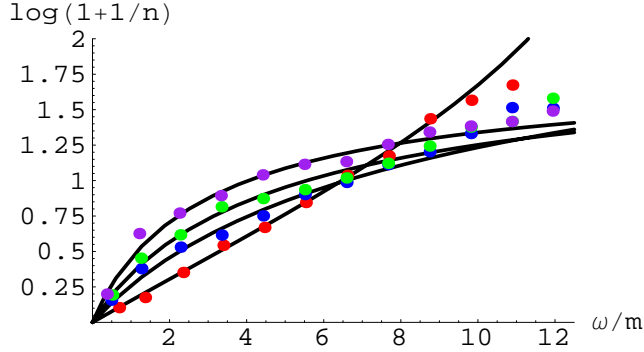


Figure 3. Particle number densities as a function of  $\omega$  at times  $tm \approx 1700$  (straight line), and 8000, 15000 and 27000 (increasingly curved lines). The drawn lines are fits with Ansatz  $n = c_0 + c_1/\omega$ . ( $Lm = 5.7$ ,  $\lambda/m^2 = 0.083$  and  $1/am = 22$ ).

over the modes.

Since the Hartree dynamics follows from a hamiltonian, one might expect that eventually equipartition sets in. To investigate this, we have run a simulation for long times, with BE-type initial conditions. The results for several times are shown in Fig. 3. The (curved) lines here are fits to the data with Ansatz  $n = c_0 + c_1/\omega$ . For times  $tm \lesssim 2000$ , the data show a BE-distribution, which was established within  $tm \lesssim 200$ . At later times  $tm \gg 2000$  one recognizes classical equipartition with temperature  $T = c_1$  and  $c_0 \approx 0$ . Since the energy is gradually distributed over particles with increasingly larger momentum range, the temperature slowly decreases.

To see the difference between our Hartree and purely classical dynamics, we have repeated the simulation of Fig. 2 (left), now using the classical e.o.m. for  $\varphi$ . As can be seen in Fig. 2 (right) the initial BE distribution with  $T = 6.7m$  evolves to equipartition much faster. Already at  $tm \approx 4200$  we find that the distribution is well represented by the classical form  $n = 3.7m/\omega$  (the curved line in Fig. 2 (right)).

Finally we try to improve the efficiency of our method. Since we have to solve for  $N$  mode functions, on a lattice with  $N$  sites, the CPU time for one time-step grows  $\propto N^2$ . However, mode functions corresponding to particles with momenta much larger than  $T$  should be irrelevant, since these particle densities are exponentially suppressed. This suggests that we can discard such modes. This is tested in Fig. 4, where we compare simulation results using all mode functions with results obtained using only a quarter of the mode functions. This corresponds with mode functions with initial plane

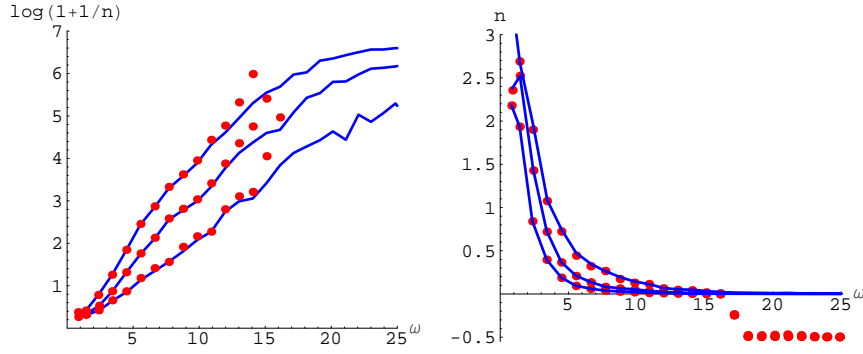


Figure 4. Hartree dynamics with all mode functions (drawn lines) and with a reduced number (32 out of 128) mode functions (dots). ( $Lm = 5.7$ ,  $\lambda/m^2 = 0.083$  and  $1/am = 22$ ).

wave energy  $\omega \lesssim 17m$ . Clearly the results for particles with significant densities  $n$  are indistinguishable. For particles with energy larger than  $\approx 17m$ , there are no longer mode functions that can provide the vacuum fluctuations and consequently the particle density defined by (6) drops to  $-1/2$ .

#### 4 Conclusion

We have demonstrated that, using our Hartree ensemble method, we can simulate quantum thermalization in a simple scalar field model in real time. Only after times much longer than typical equilibration and damping times, the approximate nature of the dynamics shows up in deviations from the BE distribution towards classical equipartition. See the contribution of Smit in these proceedings for an estimate of damping times in our model<sup>4</sup>. We have furthermore shown that these simulations can be done using a limited number of mode functions: only mode functions for particles with energies below a few times the temperature are required.

#### References

1. D. Grigoriev and V. Rubakov, Nucl. Phys. B299 (1988) 67.
2. G. Aarts, G.F. Bonini and C. Wetterich, hep-ph/0003262, hep-ph/0007357.
3. B. Mihaila, T. Athan, F. Cooper, J. Dawson and S. Habib, hep-ph/0003105.
4. M. Sallé, J. Smit and J.C. Vink, these proceedings.